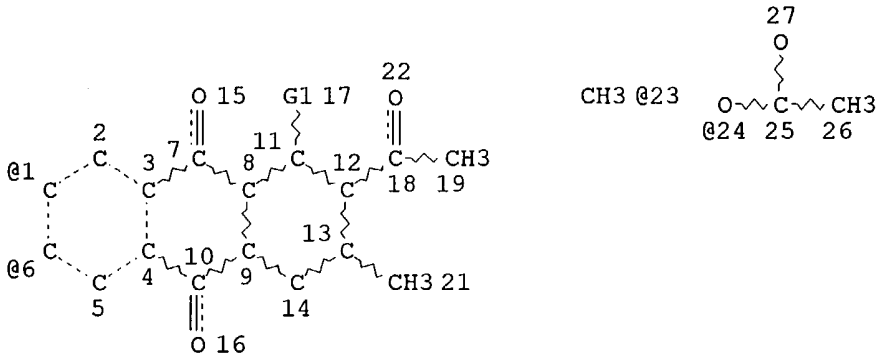
Peselev
10/761071

(FILE 'REGISTRY' ENTERED AT 11:07:55 ON 27 JUL 2004)
L1 STR

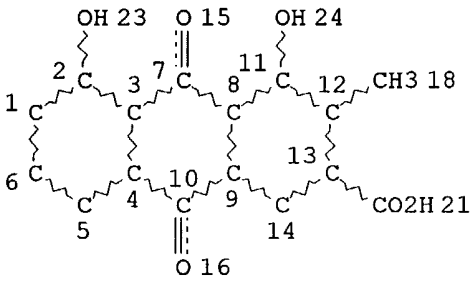


Strs.
Claims 25, 26
27 & 28

VAR G1=OH/24
VPA 23-1/6 U
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE
L4 STR



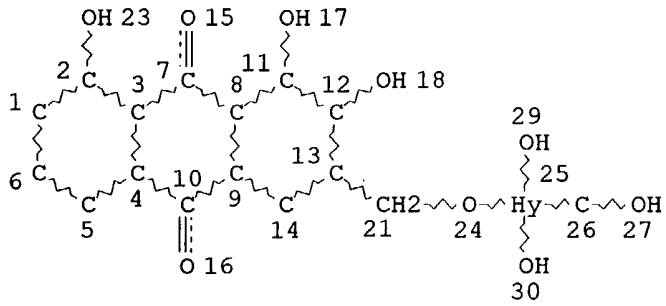
Claim 33

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
L5 STR

Searcher : Shears 571-272-2528

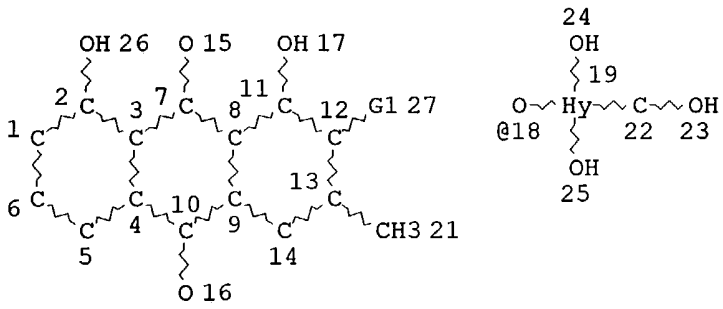


Claim 32

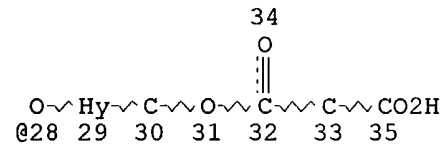
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE
L7 STR



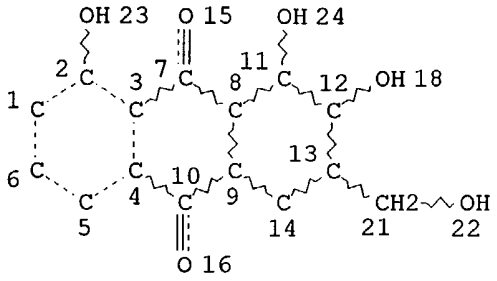
Claims 29 & 30



VAR G1=18/28
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE
L9 STR



claim 31

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE
L11 14 SEA FILE=REGISTRY SSS FUL L1 OR L7 OR L9 OR L4 OR L5

100.0% PROCESSED 86012 ITERATIONS 14 ANSWERS
SEARCH TIME: 00.00.05

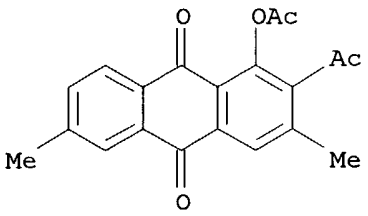
(FILE 'CAPLUS' ENTERED AT 11:19:30 ON 27 JUL 2004)
L12 17 S L11

L12 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:78682 CAPLUS
DOCUMENT NUMBER: 140:368230
TITLE: Inhibition of human tumor cell proliferation by novel anthraquinones from daylilies
AUTHOR(S): Cichewicz, Robert H.; Zhang, Yanjun; Seeram, Navindra P.; Nair, Muraleedharan G.
CORPORATE SOURCE: Department of Horticulture and National Food Safety and Toxicology Center, Bioactive Natural Products and Phytoceuticals, Michigan State University, East Lansing, MI, 48824, USA
SOURCE: Life Sciences (2004), 74(14), 1791-1799
CODEN: LIFSAK; ISSN: 0024-3205
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Daylilies (Hemerocallis) are used medicinally in eastern Asia and exts. of the plant had been shown to inhibit cell proliferation and induce cancer cells to undergo differentiation. In our studies of the constituents of Hemerocallis fulva var. Kwanzo' roots, we isolated a series of new [kwanzoquinones A (1), B (2), C (4), D (5), E (6), F (7), G (9)] and known [2-hydroxychrysophanol (3) and rhein (8)] anthraquinones. These compds. were tested in order to determine their potential roles as cancer cell growth inhibitors. Kwanzoquinones A-C and E, kwanzoquinone A and B monoacetates (1a and 2a), 2-hydroxychrysophanol, and rhein inhibited the proliferation of

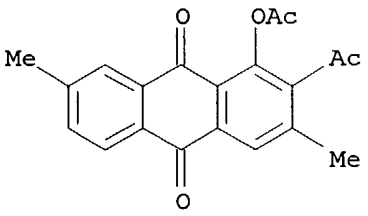
human breast, CNS, colon, and lung cancer cells with GI50 values between 1.8 to 21.1 μg/mL. However, upon exposure of the cancer cells to the GI50 concns. of the bioactive anthraquinones, most of the cancer cell lines exhibited higher than anticipated levels of cell viability. Co-incubation of the anthraquinones with vitamins C and E increased the viability of breast cancer cells. In contrast, vitamins C and E potentiated the cytotoxic effects of the anthraquinones against the colon cancer cells. None of the anthraquinones inhibited the activity of topoisomerase.

IT **479416-55-2 479416-56-3 479482-92-3,** Kwanzoquinone C **479482-93-4,** Kwanzoquinone D **479482-94-5,** Kwanzoquinone E **479482-95-6,** Kwanzoquinone F **479482-96-7,** Kwanzoquinone G
RL: NPO (Natural product occurrence); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(inhibition of human tumor cell proliferation by novel anthraquinones from daylilies)

RN 479416-55-2 CAPLUS
CN 9,10-Anthracenedione, 2-acetyl-1-(acetyloxy)-3,6-dimethyl- (9CI) (CA INDEX NAME)

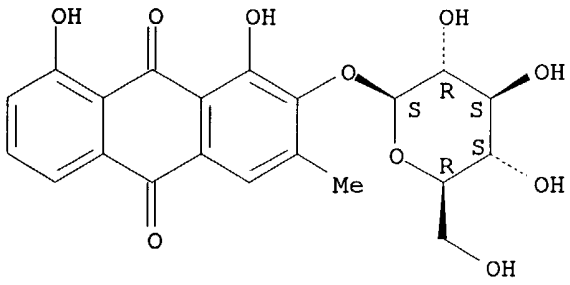


RN 479416-56-3 CAPLUS
CN 9,10-Anthracenedione, 2-acetyl-1-(acetyloxy)-3,7-dimethyl- (9CI) (CA INDEX NAME)



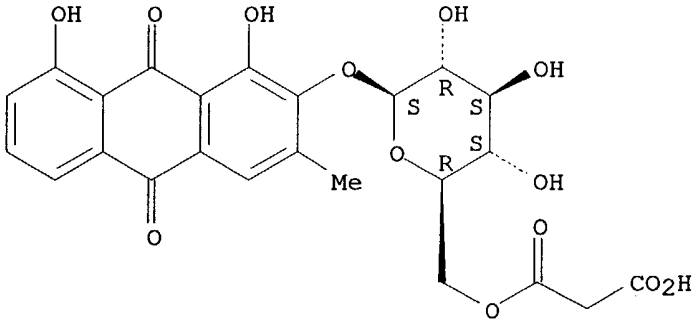
RN 479482-92-3 CAPLUS
CN 9,10-Anthracenedione, 2-(β-D-glucopyranosyloxy)-1,8-dihydroxy-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

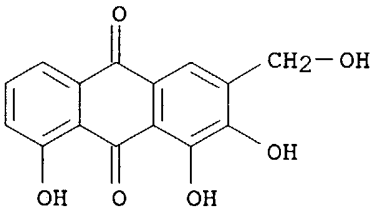


RN 479482-93-4 CAPLUS
CN 9,10-Anthracenedione, 2-[[6-O-(carboxyacetyl)-β-D-glucopyranosyl]oxy]-1,8-dihydroxy-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

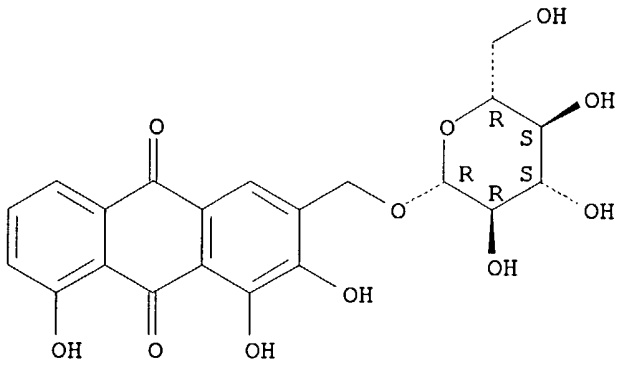


RN 479482-94-5 CAPLUS
CN 9,10-Anthracenedione, 1,2,8-trihydroxy-3-(hydroxymethyl)- (9CI) (CA INDEX NAME)

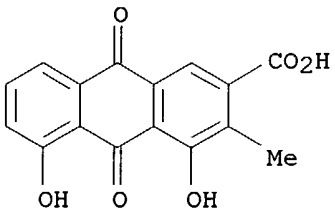


RN 479482-95-6 CAPLUS
CN 9,10-Anthracenedione, 3-[(β-D-glucopyranosyloxy)methyl]-1,2,8-trihydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

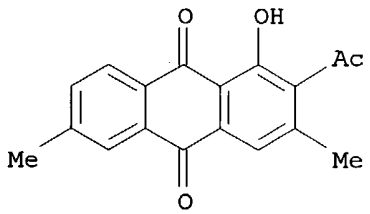


RN 479482-96-7 CAPLUS
CN 2-Anthracenecarboxylic acid, 9,10-dihydro-4,5-dihydroxy-3-methyl-9,10-dioxo- (9CI) (CA INDEX NAME)

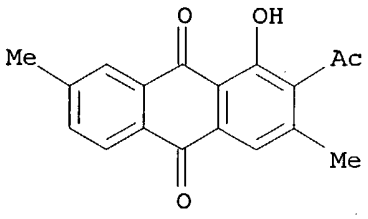


IT **479482-90-1**, Kwanzoquinone A **479482-91-2**, Kwanzoquinone B
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibition of human tumor cell proliferation by novel anthraquinones from daylilies)

RN 479482-90-1 CAPLUS
CN 9,10-Anthracenedione, 2-acetyl-1-hydroxy-3,6-dimethyl- (9CI) (CA INDEX NAME)



RN 479482-91-2 CAPLUS
CN 9,10-Anthracenedione, 2-acetyl-1-hydroxy-3,7-dimethyl- (9CI) (CA INDEX NAME)



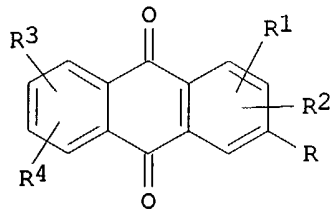
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:856025 CAPLUS
DOCUMENT NUMBER: 139:345896
TITLE: Anthelmintic anthraquinones and method of use thereof
INVENTOR(S): Cichewicz, Robert H.; Nair, Muraleedharan G. Nair; McKerrow, James H.
PATENT ASSIGNEE(S): Michigan State University, USA; The Regents of the University of California
SOURCE: PCT Int. Appl., 80 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003089577	A2	20031030	WO 2003-US11303	20030411
WO 2003089577	A3	20031231		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003229032	A1	20031211	US 2002-317906	20021212
US 2004106686	A1	20040603	US 2003-723671	20031126
US 2004116361	A1	20040617	US 2003-723672	20031126

PRIORITY APPLN. INFO.:
US 2002-372576P P 20020415
US 2002-389368P P 20020617
US 2002-317906 A 20021212

OTHER SOURCE(S): MARPAT 139:345896
GI



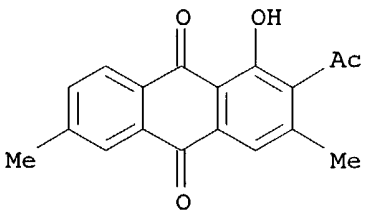
I

AB Anthraquinones are described which are anthelmintic and in particular, are useful in compns. for inhibiting Schistosoma sp. In vitro or in vivo. The preferred anthraquinones have the formula (I) wherein R1, R2, R3, and R4 are each hydrogen, hydroxy, halogen, alkyl, substituted alkyl, alkene, substituted alkene, alkyne, aryl, substituted aryl, cyclic, substituted cyclic, acid group, carbohydrate, or combination thereof, R is a group containing 1 to 12 carbons such as Me, alkyl, substituted alkyl, aldehyde, hydroxy, hydroxymethyl, acid group, 15 carbohydrate, or combination thereof, and the halogen X is I, F, Br, or Cl. The isolation and characterization of anthraquinones from the roots of daylilies (Hemerocallis fulva) is described.

IT **479482-90-1P**, Kwanzoquinone A **479482-91-2P**, Kwanzoquinone B **479482-92-3P**, Kwanzoquinone C **479482-93-4P**, Kwanzoquinone D **479482-94-5P**, Kwanzoquinone E **479482-95-6P**, Kwanzoquinone F **479482-96-7P**, Kwanzoquinone G
RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)
(anthelmintic anthraquinones in relation to isolation from daylily Hemerocallis)

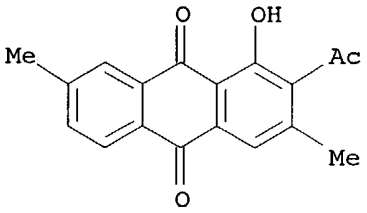
RN 479482-90-1 CAPLUS

CN 9,10-Anthracenedione, 2-acetyl-1-hydroxy-3,6-dimethyl- (9CI) (CA INDEX NAME)



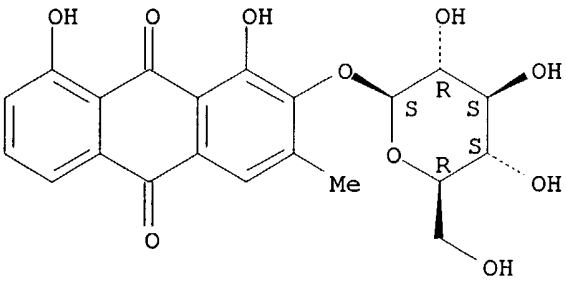
RN 479482-91-2 CAPLUS

CN 9,10-Anthracenedione, 2-acetyl-1-hydroxy-3,7-dimethyl- (9CI) (CA INDEX NAME)



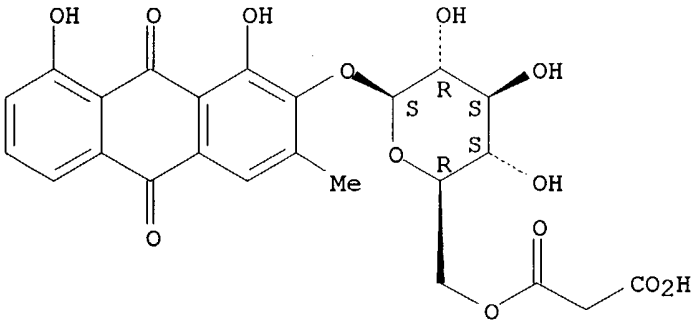
RN 479482-92-3 CAPLUS
CN 9,10-Anthracenedione, 2-(β-D-glucopyranosyloxy)-1,8-dihydroxy-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

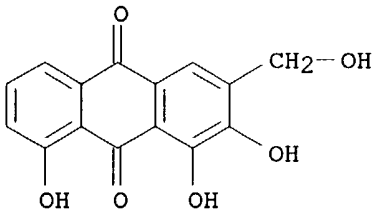


RN 479482-93-4 CAPLUS
CN 9,10-Anthracenedione, 2-[[6-O-(carboxyacetyl)-β-D-glucopyranosyl]oxy]-1,8-dihydroxy-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

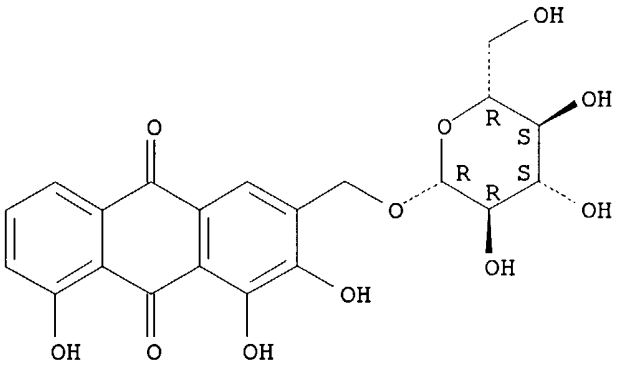


RN 479482-94-5 CAPLUS
CN 9,10-Anthracenedione, 1,2,8-trihydroxy-3-(hydroxymethyl)- (9CI) (CA INDEX NAME)

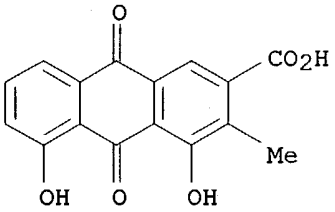


RN 479482-95-6 CAPLUS
CN 9,10-Anthracenedione, 3-[(β-D-glucopyranosyloxy)methyl]-1,2,8-trihydroxy- (9CI) (CA INDEX NAME)

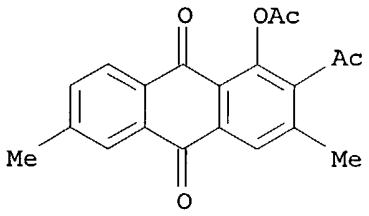
Absolute stereochemistry. Rotation (-).



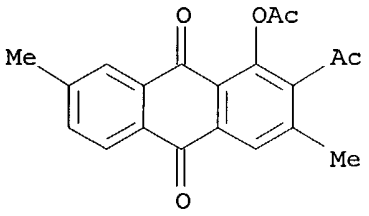
RN 479482-96-7 CAPLUS
CN 2-Anthracenecarboxylic acid, 9,10-dihydro-4,5-dihydroxy-3-methyl-9,10-dioxo- (9CI) (CA INDEX NAME)



IT **479416-55-2 479416-56-3**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(anthelmintic anthraquinones in relation to isolation from daylily Hemerocallis)
RN 479416-55-2 CAPLUS
CN 9,10-Anthracenedione, 2-acetyl-1-(acetyloxy)-3,6-dimethyl- (9CI) (CA INDEX NAME)



RN 479416-56-3 CAPLUS
CN 9,10-Anthracenedione, 2-acetyl-1-(acetyloxy)-3,7-dimethyl- (9CI) (CA INDEX NAME)



L12 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:856024 CAPLUS
DOCUMENT NUMBER: 139:341716
TITLE: Anticancer anthraquinones from Hemerocallis fulva
INVENTOR(S): Nair, Muraleedharan G. Nair; Cichewicz, Robert H.; Seeram, Navindra P.; Zhang, Yanjun
PATENT ASSIGNEE(S): Michigan State University, USA
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003089576	A2	20031030	WO 2003-US11302	20030411
WO 2003089576	A3	20031231		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM,

GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
US 2003229032 A1 20031211 US 2002-317906 20021212
PRIORITY APPLN. INFO.: US 2002-372576P P 20020415
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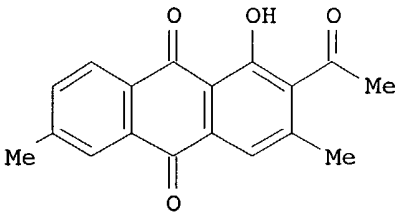
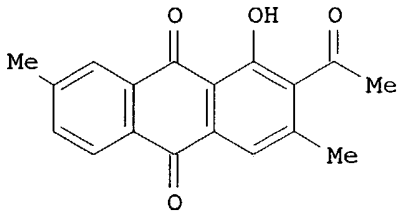
GI



I



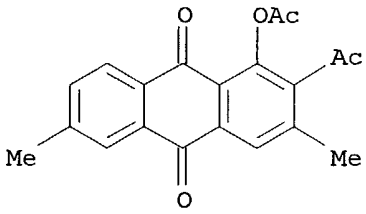
II

AB Anthraquinones are described which have anticancer or antitumor activity and which are useful for inhibiting cancer cells and cells comprising tumors in vitro or in vivo. Anthraquinones such as kwanzoquinones A (I) and B (II) along with six other derivs. were isolated from Hemerocallis fulva plants and their antitumor activity determined

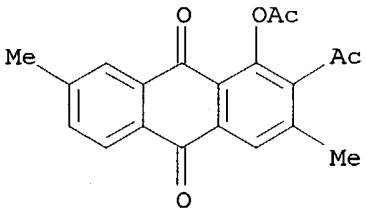
IT **479416-55-2**, 9,10-Anthracenedione, 2-acetyl-1-acetyloxy-3,6-dimethyl- **479416-56-3**, 9,10-Anthracenedione, 2-acetyl-1-acetyloxy-3,7-dimethyl- **479482-90-1**, Kwanzoquinone A **479482-91-2**, Kwanzoquinone B **479482-92-3**, Kwanzoquinone C **479482-94-5**, Kwanzoquinone E
RL: NPO (Natural product occurrence); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(anticancer anthraquinones from Hemerocallis fulva)

RN 479416-55-2 CAPLUS

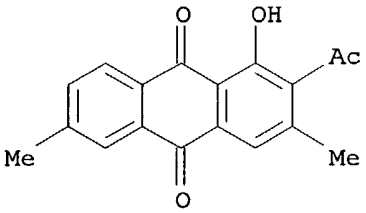
CN 9,10-Anthracenedione, 2-acetyl-1-(acetyloxy)-3,6-dimethyl- (9CI) (CA INDEX NAME)



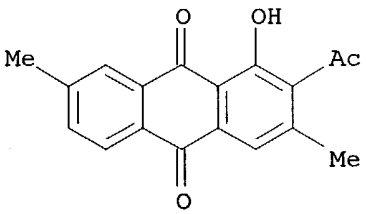
RN 479416-56-3 CAPLUS
CN 9,10-Anthracenedione, 2-acetyl-1-(acetyloxy)-3,7-dimethyl- (9CI) (CA INDEX NAME)



RN 479482-90-1 CAPLUS
CN 9,10-Anthracenedione, 2-acetyl-1-hydroxy-3,6-dimethyl- (9CI) (CA INDEX NAME)

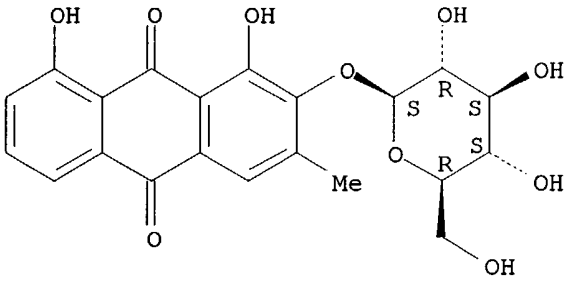


RN 479482-91-2 CAPLUS
CN 9,10-Anthracenedione, 2-acetyl-1-hydroxy-3,7-dimethyl- (9CI) (CA INDEX NAME)

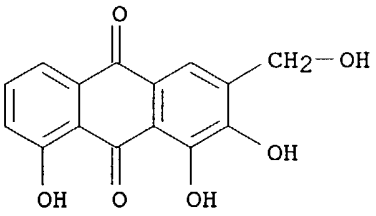


RN 479482-92-3 CAPLUS
CN 9,10-Anthracenedione, 2-(β-D-glucopyranosyloxy)-1,8-dihydroxy-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 479482-94-5 CAPLUS
CN 9,10-Anthracenedione, 1,2,8-trihydroxy-3-(hydroxymethyl)- (9CI) (CA INDEX NAME)



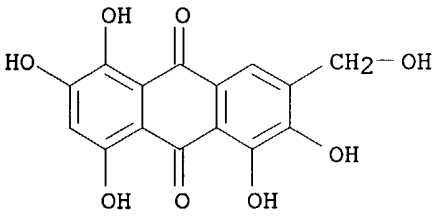
L12 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:459324 CAPLUS
DOCUMENT NUMBER: 140:106640
TITLE: Fungal metabolite screening: database of 474 mycotoxins and fungal metabolites for dereplication by standardized liquid chromatography-UV-mass spectrometry methodology
AUTHOR(S): Nielsen, Kristian Fog; Smedsgaard, Jorn
CORPORATE SOURCE: BioCentrum-DTU, Mycology Group, Technical University of Denmark, Lyngby, DK-2800, Den.
SOURCE: Journal of Chromatography, A (2003), 1002(1-2), 111-136
CODEN: JCRAEY; ISSN: 0021-9673
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A standardized LC-UV-MS micro-scale method for screening of fungal metabolites and mycotoxins in culture exts. is presented. The paper includes data for detection and dereplication of >400 fungal metabolites to facilitate detection and identification when stds. are not available. The data also shows the types of components that can be analyzed by pos. electrospray (ESI+) mass spectrometry (MS)

along with common fragments and adducts of these, as well as giving suggestions on whether UV or ESI+-MS methods should be used. Examples of dereplication of penitrems and macro-cyclic trichothecenes, and detection of several novel compds. are shown. This was done by UV spectroscopy combined with accurate mass determination of adduct and fragment ions obtained by high-resolution orthogonal time-of-flight MS.

IT **10089-00-6**, Asperthecin
RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)
(database of 474 mycotoxins and fungal metabolites for dereplication by standardized liquid chromatog.-UV-mass spectrometry methodol.)

RN 10089-00-6 CAPLUS

CN 9,10-Anthracenedione, 1,2,5,6,8-pentahydroxy-3-(hydroxymethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 71 THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:788802 CAPLUS

DOCUMENT NUMBER: 138:52682

TITLE: Kwanzoquinones A-G and other constituents of Hemerocallis fulva 'Kwanzo' roots and their activity against the human pathogenic trematode Schistosoma mansoni

AUTHOR(S): Cichewicz, Robert H.; Lim, Kee-Chong; McKerrow, James H.; Nair, Muraleedharan G.

CORPORATE SOURCE: Department of Horticulture and National Food Safety and Toxicology Center, Bioactive Natural Products and Phytoceuticals, Michigan State University, East Lansing, MI, 48824, USA

SOURCE: Tetrahedron (2002), 58(42), 8597-8606
CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

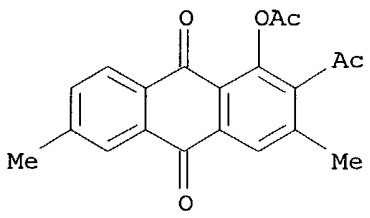
LANGUAGE: English

AB Schistosomiasis is a debilitating disease caused by parasitic trematodes of the genus Schistosoma that afflicts 200 million people worldwide. Daylilies (Hemerocallis spp.) have been used in Asia for the treatment of schistosomiasis; however, the active principles have not been fully characterized. In our studies of Hemerocallis fulva Kwanzo' Kaempfer roots, we have isolated seven new anthraquinones, kwanzoquinones A (1), B (2), C (4), D (5), E (6), F

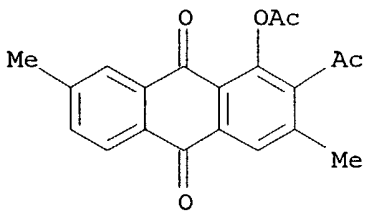
(7), and G (9), two known anthraquinones, 2-hydroxychrysophanol (3) and rhein (8), one new naphthalene glycoside, 5-hydroxydianellin (11), one known naphthalene glycoside, dianellin (10), one known flavone, 6-methylluteolin (12), and α-tocopherol. The structures of the compds. were elucidated by spectroscopic and chemical methods. Compds. 1-11 and the monoacetates of kwanzoquinones A and B, 1a and 2a, resp., were tested for their activity against multiple life-stages of Schistosoma mansoni. Compound 3 immobilized all cercariae within 15 s at 3.1 μg/mL. However, upon removal of the compound, 20% of the immobilized cercariae recovered after 24 h. In contrast, compound 6 immobilized cercariae within 12-14 min at 25 μg/mL. Following removal of the compound, all cercariae died within 24 h. The adult worms were also immobilized within 16 h by compds. 3 and 6 at 50 μg/mL. None of the compds. had an effect on the schistosomula stage.

IT **479416-55-2P 479416-56-3P 479482-90-1P,** Kwanzoquinone A **479482-91-2P,** Kwanzoquinone B **479482-92-3P,** Kwanzoquinone C **479482-93-4P,** Kwanzoquinone D **479482-94-5P,** Kwanzoquinone E **479482-95-6P,** Kwanzoquinone F **479482-96-7P,** Kwanzoquinone G
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(kwanzoquinones A-G of Hemerocallis fulva roots and their activity against Schistosoma mansoni)

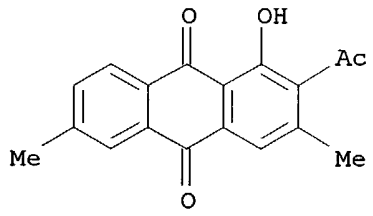
RN 479416-55-2 CAPLUS
CN 9,10-Anthracenedione, 2-acetyl-1-(acetyloxy)-3,6-dimethyl- (9CI) (CA INDEX NAME)



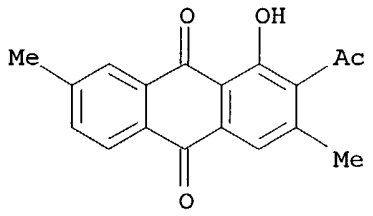
RN 479416-56-3 CAPLUS
CN 9,10-Anthracenedione, 2-acetyl-1-(acetyloxy)-3,7-dimethyl- (9CI) (CA INDEX NAME)



RN 479482-90-1 CAPLUS
CN 9,10-Anthracenedione, 2-acetyl-1-hydroxy-3,6-dimethyl- (9CI) (CA INDEX NAME)

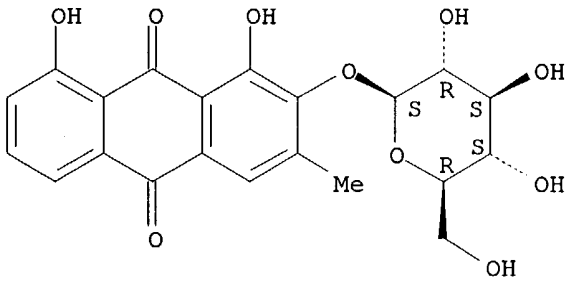


RN 479482-91-2 CAPLUS
CN 9,10-Anthracenedione, 2-acetyl-1-hydroxy-3,7-dimethyl- (9CI) (CA INDEX NAME)



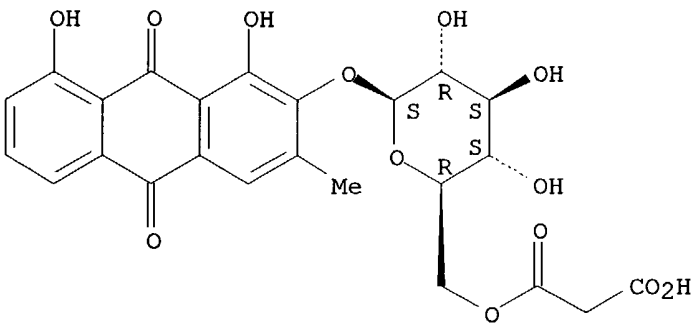
RN 479482-92-3 CAPLUS
CN 9,10-Anthracenedione, 2-(β-D-glucopyranosyloxy)-1,8-dihydroxy-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

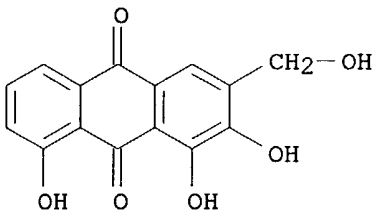


RN 479482-93-4 CAPLUS
CN 9,10-Anthracenedione, 2-[[6-O-(carboxyacetyl)-β-D-glucopyranosyl]oxy]-1,8-dihydroxy-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

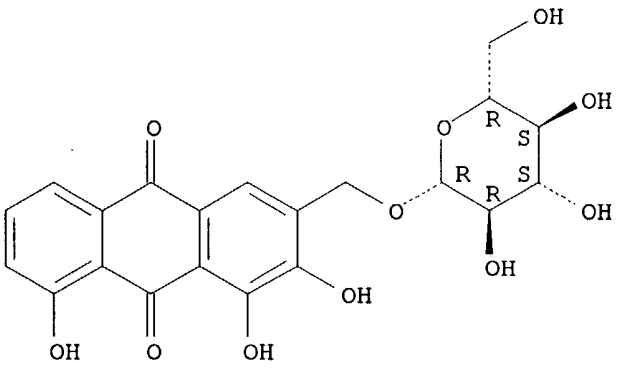


RN 479482-94-5 CAPLUS
CN 9,10-Anthracenedione, 1,2,8-trihydroxy-3-(hydroxymethyl)- (9CI) (CA INDEX NAME)

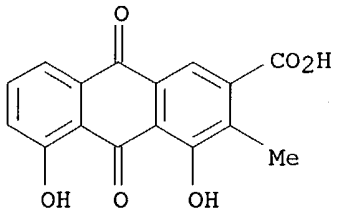


RN 479482-95-6 CAPLUS
CN 9,10-Anthracenedione, 3-[(β-D-glucopyranosyloxy)methyl]-1,2,8-trihydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 479482-96-7 CAPLUS
CN 2-Anthracenecarboxylic acid, 9,10-dihydro-4,5-dihydroxy-3-methyl-9,10-dioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

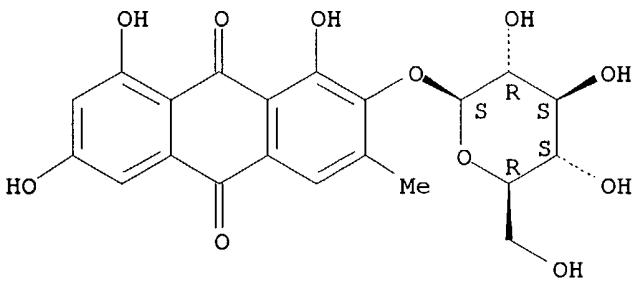
L12 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:785052 CAPLUS
DOCUMENT NUMBER: 130:110478
TITLE: Alaternin glucoside isomer from Cassia tora
AUTHOR(S): Lee, Hee Jung; Choi, Jae Sue; Jung, Jee Hyung; Kang, Sam Sik
CORPORATE SOURCE: Dept. of Food and Life Science, Pukyong National University, Pusan, 608-737, S. Korea
SOURCE: Phytochemistry (1998), 49(5), 1403-1404
CODEN: PYTCAS; ISSN: 0031-9422
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB From the seeds of Cassia tora, an anthraquinone glucoside was isolated and characterized as alaternin 2-O-β-D-glucopyranoside.

IT **219607-92-8P**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(isolation of alaternin glucoside isomer from Cassia tora)

RN 219607-92-8 CAPLUS
CN 9,10-Anthracenedione, 2-(β-D-glucopyranosyloxy)-1,6,8-trihydroxy-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

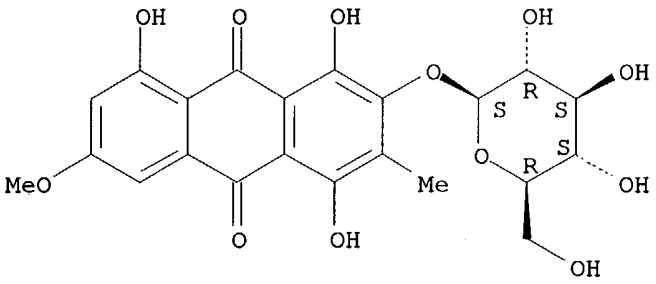


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN

THE RE FORMAT

L12 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:212583 CAPLUS
DOCUMENT NUMBER: 120:212583
TITLE: Anthraquinone-O-β-D-glucosides from Cassia grandis
AUTHOR(S): Siddiqui, Ibadur Rahman; Singh, Mithiles; Gupta, Dipti; Singh, Jagdamba
CORPORATE SOURCE: Dep. Chem., Univ. Allahabad, 211 002, India
SOURCE: Natural Product Letters (1993), 2(2), 83-90
CODEN: NPLEEF; ISSN: 1057-5634
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Chemical investigation of the seeds of Cassia grandis yielded three new anthraquinone glucosides, 1,2,4,8-tetrahydroxy-6-methoxy-3-methylanthraquinone 2-O-β-D-glucopyranoside, 3-hydroxy-6,8-dimethoxy-2-methylanthraquinone 3-O-β-D-glucopyranoside and 1,3-dihydroxy-6,7,8-trimethoxyanthraquinone 3-O-β-D-glucopyranoside. The structures of these glucosides were elucidated by a combination of chemical and spectroscopic methods and finally by their syntheses.
IT **144828-10-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and isolation of, from Cassia grandis)
RN 144828-10-4 CAPLUS
CN 9,10-Anthracenedione, 3-(β-D-glucopyranosyloxy)-1,4,5-trihydroxy-7-methoxy-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:3859 CAPLUS
DOCUMENT NUMBER: 118:3859
TITLE: Isolation, characterization and synthesis of three new anthraquinone glycosides from Cassia grandis
AUTHOR(S): Singh, M.; Siddiqui, I. R.; Gupta, D.; Singh, J.
CORPORATE SOURCE: Dep. Chem., Univ. Allahabad, Allahabad, India
SOURCE: Polish Journal of Chemistry (1992), 66(3), 469-75
CODEN: PJCHDQ; ISSN: 0137-5083
DOCUMENT TYPE: Journal

LANGUAGE: English

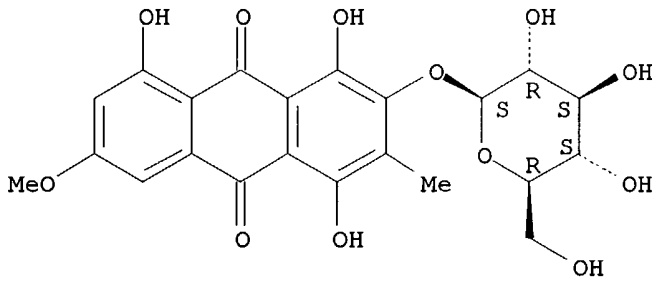
AB From the seeds of Cassia grandis, three glycosides, namely 2-O-β-D-glucopyranosyl-1,2,4,8-tetrahydroxy-6-methoxy-3-methylanthraquinone, 3-O-β-D-glucopyranosyl-3-hydroxy-6,8-dimethoxy-2-methylanthraquinone and 3-O-β-D-glucopyranosyl-1,3-dihydroxy-6,7,8-trimethoxy-2-methylanthraquinone have been isolated. The structures were determined by spectroscopic methods and confirmed by synthesis.

IT **144828-10-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(from Cassia grandis, isolation and hydrolysis of)

RN 144828-10-4 CAPLUS

CN 9,10-Anthracenedione, 3-(β-D-glucopyranosyloxy)-1,4,5-trihydroxy-7-methoxy-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1987:592376 CAPLUS

DOCUMENT NUMBER: 107:192376

TITLE: Standardized high-performance liquid chromatography of 182 mycotoxins and other fungal metabolites based on alkylphenone retention indexes and UV-VIS spectra (diode array detection)

AUTHOR(S): Frisvad, Jens; Thrane, Ulf

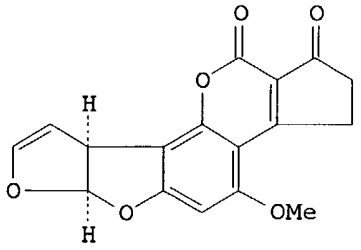
CORPORATE SOURCE: Dep. Biotechnol., Tech. Univ. Denmark, Lyngby, DK-2800, Den.

SOURCE: Journal of Chromatography (1987), 404(1), 195-214
CODEN: JOCRAM; ISSN: 0021-9673

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



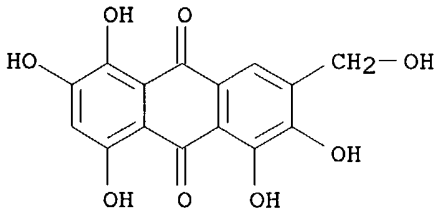
I

AB A general standardized method for the anal. of mycotoxins and other fungal secondary metabolites was developed, based on HPLC with an alkylphenone retention index and photodiode-array detection combined with TLC in 2 different eluents. Each fungal secondary metabolite is characterized by its bracketed alkylphenone retention time index, its UV-VIS absorption maximum and its retardation factors relative to griseofulvin in 2 TLC eluents. This system is effective for the comparison of chemotaxonomic data in different labs. and for a precise identification of fungi based on organic solvent exts. of fungal cultures. All important groups of mycotoxins and other fungal secondary metabolites could be detected in the HPLC system described and data are listed for 182 metabolites. The fungal secondary metabolites separated and characterized include aflatoxin B1 (I), B2, G1 and G2, ochratoxin A, citrinin, penicillin acid, viomellein, penitrem A, patulin, sterigmatocystin, alternariol, tenuazonic acid, trichothecenes, roquefortines, fusarin C, zearalenone, PR-toxin, citreoviridin, viridicatumtoxin, verruculogen, rugulosin, cyclopiazonic acid, penicillin G, and many other alkaloids, polyketides, and terpenes.

IT **10089-00-6**, Asperthecin
RL: ANT (Analyte); ANST (Analytical study)
(HPLC and TLC determination of)

RN 10089-00-6 CAPLUS

CN 9,10-Anthracenedione, 1,2,5,6,8-pentahydroxy-3-(hydroxymethyl)- (9CI) (CA INDEX NAME)



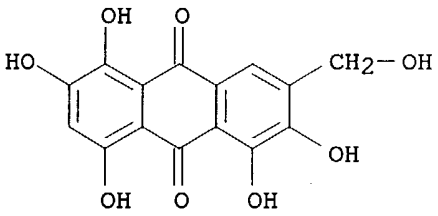
L12 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1987:436247 CAPLUS
DOCUMENT NUMBER: 107:36247
TITLE: High-performance liquid chromatographic determination of profiles of mycotoxins and

other secondary metabolites
AUTHOR(S): Frisvad, Jens C.
CORPORATE SOURCE: Dep. Biotechnol. Food Technol., Tech. Univ. Denmark, Lyngby, DK-2800, Den.
SOURCE: Journal of Chromatography (1987), 392, 333-47
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A reversed-phase HPLC determination of profiles of mycotoxins and other fungal secondary metabolites was developed. Penicillium, Aspergillus, And Fusarium polyketides, terpenes, and alkaloids were emphasized. In a gradient elution, using H2O-MeCN containing 0.05% CF3COOH, 134 secondary metabolites were eluted evenly with retention times of 1.08-34.48 min. Metabolites with the same retention time were usually not produced by the same species. As UV detection at 254 nm was used, some mycotoxins (type A trichothecenes, viridicatumtoxin, peptide-like compds., and xanthomegnin) could not be detected. The method appears to be valuable for chemotaxonomic studies of fungi. Unpurified concentrated CHCl3-MeOH exts. of petri dish cultures analyzed by the proposed method presented gave species-specific characteristic profiles of known and unknown secondary metabolites and mycotoxins.

IT **10089-00-6**
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of, from fungi)

RN 10089-00-6 CAPLUS
CN 9,10-Anthracenedione, 1,2,5,6,8-pentahydroxy-3-(hydroxymethyl)- (9CI) (CA INDEX NAME)



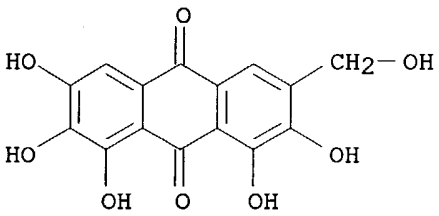
L12 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1984:506729 CAPLUS
DOCUMENT NUMBER: 101:106729
TITLE: Separation and identification of naturally occurring anthraquinones by capillary gas chromatography and gas chromatography-mass spectrometry
AUTHOR(S): Van Eijk, G. W.; Roeijmans, H. J.
CORPORATE SOURCE: Centraalbur. Schimmelcult., Baarn, 3740 AG, Neth.
SOURCE: Journal of Chromatography (1984), 295(2), 497-502
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Trimethylsilyl ethers of naturally occurring anthraquinones were prepared with a mixture of N-trimethylsilylimidazole, N,O-bis(trimethylsilyl)acetamide, and trimethylchlorosilane and analyzed directly by gas chromatog. (GC) on a wall-coated open-tubular (WCOT) fused-silica capillary column coated with CP-sil 5 CB (N carrier gas; temperature programmed) or by GC-mass spectroscopy (MS) on a CP-sil 5 WCOT fused-silica capillary column (He carrier gas; temperature programmed). The GC retention times and MS data of 37 trimethylsilylated anthraquinones are tabulated. The method requires only 25 min and low oven end temperature, and the small mol. ions can be detected with a low-cost quadrupole mass spectrometer.

IT **481-68-5**
RL: ANT (Analyte); ANST (Analytical study)
(detection of, by capillary gas chromatog.-mass spectroscopy)

RN 481-68-5 CAPLUS

CN 9,10-Anthracenedione, 1,2,3,7,8-pentahydroxy-4-(hydroxymethyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1963:39865 CAPLUS
DOCUMENT NUMBER: 58:39865
ORIGINAL REFERENCE NO.: 58:6759d-f
TITLE: Synthesis of polyhydroxyanthraquinones related to asperthecin
AUTHOR(S): Birkinshaw, J. H.; Gourlay, Rachel
CORPORATE SOURCE: Univ. London
SOURCE: Journal of the Chemical Society, Abstracts (1963) 716-20
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 58:39865

GI For diagram(s), see printed CA Issue.

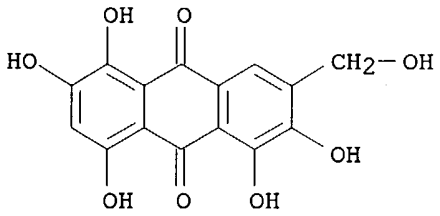
AB In the presence of sulfuric acid 2-(2-hydroxy-4,5-dimethoxybenzoyl)-3,4-dimethoxybenzoic acid undergoes the Hayashi rearrangement (CA 24, 5033) to yield 6-(2-hydroxy-4,5-dimethoxybenzoyl) - 2,3-dimethoxybenzoic acid. The latter, on ring closure and demethylation, gives 1,3,4,5,6-pentahydroxyanthraquinone (I), the structure of which is confirmed by synthesis from 1,2,4-trimethoxybenzene and opianic acid.

IT **10089-00-6**, Asperthecin
(polyhydroxyanthraquinones related to)

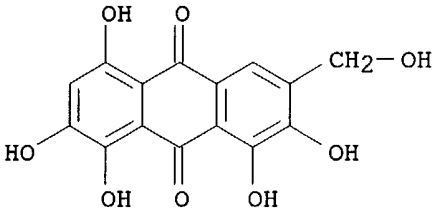
RN 10089-00-6 CAPLUS

CN 9,10-Anthracenedione, 1,2,5,6,8-pentahydroxy-3-(hydroxymethyl)-

(9CI) (CA INDEX NAME)



IT **92439-43-5**, Anthraquinone, 1,2,5,7,8-pentahydroxy-3-(hydroxymethyl)-
(preparation of)
RN 92439-43-5 CAPLUS
CN Anthraquinone, 1,2,5,7,8-pentahydroxy-3-(hydroxymethyl)- (7CI) (CA INDEX NAME)



L12 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1962:45896 CAPLUS
DOCUMENT NUMBER: 56:45896
ORIGINAL REFERENCE NO.: 56:8653i,8654a-i,8655a
TITLE: Biochemistry of microorganisms. CIX. The structure of asperthecin
AUTHOR(S): Birkinshaw, J. H.; Gourlay, Rachel
CORPORATE SOURCE: Univ. London
SOURCE: Biochemical Journal (1961), 81, 618-22
CODEN: BIJOAK; ISSN: 0264-6021
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. CA 55, 7537b. Several new derivs. of asperthecin (I) were prepared Triacetylasperthecin: I was refluxed with Ac2O 12 min., and cooled to yield crystals, m. 284-50° (Ac2O), yield 0.08 g. from 0.1 g. of I. Tetraacetylasperthecin: the mother liquors from the above when poured into H2O gave a precipitate, m. 251-3° (decomposition) (AcOH), yield 0.02 g., which can be improved by refluxing I with Ac2O 20 min. Asperthecic acid pentaacetate: 0.2 g. I, 1 g. H3BO3, 0.5 g. NaNO3 and 25 ml. concentrated H2SO4 was heated rapidly to 180°, cooled to 145° and maintained at 145° 80 min. The cooled solution was poured into 250 ml. H2O and heated to boiling to coagulate the product, the precipitate collected and dried, the crude material acetylated by heating with 5 ml. Ac2O and 0.1 ml.

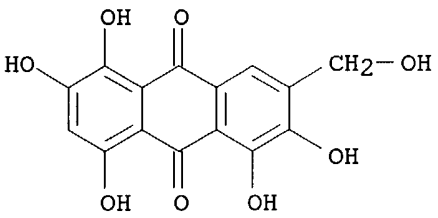
concentrated H_2SO_4 at 90° 5 min., the solution cooled, and poured into H_2O to precipitate the product, m. 218-20° (decomposition) (MeOH), yield 0.05 g. Asperthecic acid: the pentaacetate was hydrolyzed by refluxing with 5 ml. MeOH containing 0.15 ml. concentrated H_2SO_4 1 hr. to give the product, m. above 350° (decomposition) (MeOH), yield 30 mg. from 60 mg. starting material. Decarboxyasperthicic acid: 0.35 g. asperthecic acid, 15 ml. quinoline, and 0.2 g. Cu chromite was heated to 200° in a current of N 7.5 hrs., the cooled solution added to 250 ml. 2N HCl, the precipitate collected, dried, and extracted with MeOH, and the MeOH solution evaporated to 200 ml. and chromatographed on a column of $CaCO_3$ with EtOH as the eluent. The column was removed and cut into 3 portions, orange, pink, and violet. Each portion was dissolved in 5N HCl, the solns. heated to boiling and cooled, and the anthraquinone fractions filtered off and dried. Purification of fractions 2 and 3 by acetylation gave the acetyl derivs., m. 242-3°, undepressed when mixed with each other or with 3,4,5,7,8-pentaacetoxyanthraquinone. The acetate was hydrolyzed by refluxing 1.5 hrs. with 5 ml. MeOH and 0.1 ml. concentrated H_2SO_4 to give 3,4,5,7,8-pentahydroxyanthraquinone, red needles, m. 353-4°. Several syntheses were described. Hemipinic anhydride dissolved in m-methoxyphenol was heated at 70-5° with $AlCl_3$ 6 hrs. After standing overnight the red material was treated with ice and 2N HCl, the mixture extracted with Et_2O, the Et_2O solution washed with $NaHCO_3$ solution, and the $NaHCO_3$ extract acidified to produce a resinous material which was dissolved in Et_2O and crystallized to yield 2.2 g. 2-(2-hydroxy-4-methoxybenzoyl)-3,4-dimethoxybenzoic acid (II), m. 211-12°, from 5 g. starting material. II was dissolved in H_2O containing NaOH (1.33 g./20 ml.) to which was added 1.80 g. $K_2S_2O_8$. After 4 days at room temperature the deep-red solution was made faintly acid to Congo red with 5N H_2SO_4, 1.23 g. of the unchanged acid was collected by filtration, and the filtrate made strongly acid with HCl (10.0 ml.) to yield crystalline 2-(2,5-dihydroxy-4-methoxybenzoyl)-3,4-dimethoxybenzoic acid (III), m. 261-2° (decomposition). III (0.15 g.) was dissolved in acetone (20 ml.) to which 1 g. K_2CO_3 and 1.0 ml. dimethyl sulfate were added and the solution refluxed 7 hrs., kept overnight, refluxed an addnl. 7 hrs. with 1.0 ml. Me_2SO_4, the cooled solution filtered, and the acetone evaporated The residual oil was suspended in 25 ml. 2N NaOH and 5 ml. aqueous 2N NH_3 added, and the solution refluxed 2 hrs. to hydrolyze the ester, cooled, acidified, and extracted with Et_2O to give 0.032 g. 3,4-dimethoxy-2-(2,4,5-trimethoxybenzoyl)benzoic acid (IV), crystallized from the extract, m. 230-1°. II (1.1 g.), 12 ml. quinoline, and 0.4 g. Cu chromite were heated at 190-200° under the same conditions as for the decarboxylation of asperthecic acid 4 hrs. (80% completion), the cooled solution poured into 100 ml. 2N HCl, the mixture extracted with Et_2O, from which was crystallized 3,5-dimethoxyxanthone, m. 170-1°. Hemipinic acid dissolved in 1,2,4-trimethoxybenzene was treated with $AlCl_3$ 5.5 hrs. at 75-80°, the product warmed with 2N HCl, cooled, and extracted with Et_2O, and the Et_2O extract shaken with $NaHCO_3$. A crystalline solid separated from the Et_2O to give 3,4-dimethoxy-1,2-bis(2,4,5-trimethoxybenzoyl)benzene, m. 176°. The resinous product obtained on acidification of the $NaHCO_3$ solution was dissolved in Et_2O from which crystallized

2-(2-hydroxy-4,5-dimethoxybenzoyl)-3,4-dimethoxybenzoic acid (V), m. 225°, yield 0.75 g. from 2 g. starting material. 2-(2,5-Dimethoxy-4-methoxybenzoyl)-3,4-dimethoxybenzoic acid (VI), m. 230-1°, was prepared by the method used for the methylation of III. V was decarboxylated as above to yield 2,3,5-trimethoxyxanthone, m. 232-5°. AlCl3 (5 g.) and 1 g. NaCl were fused at 180°, cooled to 120°, 0.56 g. V added, the mixture heated at 190° 5 min., cooled with ice, mixed with 20 ml. concentrated HCl, diluted with 400 ml. H2O, brought to a boil, and the precipitate filtered off, washed, and dried. The product was heated 10 min. at 70-80° with 5 ml. Ac2O containing 0.1 ml. concentrated H2SO4. On cooling, 3,4,5,7,8-pentaacetoxyanthraquinone crystallized, m. 241-2°, yield 0.39 g. Refluxing this compound with 25 ml. MeOH containing 0.75 ml. concentrated H2SO4 yielded 3,4,5,7,8-pentahydroxyanthraquinone, m. 353-5°, yield 0.15 g. from 0.27 g. starting material. Asperthecin is represented by the structure 3,4,5,7,8-pentahydroxy-2-hydroxymethylanthraquinone.

IT **10089-00-6**, Anthraquinone, 1,2,5,6,8-pentahydroxy-3-(hydroxymethyl)-
(as structure of asperthecin)

RN 10089-00-6 CAPLUS

CN 9,10-Anthracenedione, 1,2,5,6,8-pentahydroxy-3-(hydroxymethyl)- (9CI) (CA INDEX NAME)



(structure of

L12 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1958:6313 CAPLUS

DOCUMENT NUMBER: 52:6313

ORIGINAL REFERENCE NO.: 52:1131a-d

TITLE: Biochemistry of microorganisms. CI. The coloring matters of species of the Aspergillus nidulans group. 2. Further observations on the structure of asperthecin

AUTHOR(S): Neelakantan, S.; Pocker, Anna; Raistrick, H.

CORPORATE SOURCE: Univ. London

SOURCE: Biochemical Journal (1957), 66, 234-7
CODEN: BIJOAK; ISSN: 0264-6021

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

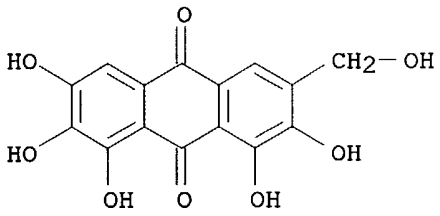
AB cf. C.A. 51, 6756b. Asperthecin has been shown to be either 3,4,5,6,7-pentahydroxy-2-hydroxymethylanthraquinone or 3,4,5,7,8-pentahydroxy-2-hydroxymethylanthraquinone. It has been confirmed that full methylation of polyhydroxyanthroquinones with ethereal diazomethane is greatly facilitated by the addition of MeOH to

the methylation mixture 4-Carboxy-3,6-dimethoxyphthalic anhydride has been synthesized from 3,6-dimethoxy-4-mehylphthalic anhydride by refluxing in 0.5N NaOH with 1% (weight/volume) KMnO4. 5-Carboxy-3,4-dimethoxyphthalic acid was synthesized from 5-methylmeconin (synthesis given) by refluxing in N NaOH with continuous addition of KMnO4. The corresponding anhydride was prepared by heating the acid above its m.p. 15 min. 3,4-Dimethoxy-5-methylphthalic acid was synthesized from 5-methylmeconin by oxidation with KMnO4 at room temperature overnight. The anhydride was prepared by heating the acid to sublimation and recovering the sublimate. 5-Carboxy-3,4-dimethylphthalic anhydride has been identified as an oxidation product of asperthecin tetra- and penta-Me ethers.

IT **481-68-5**, Anthraquinone, 1,2,3,7,8-pentahydroxy-6-(hydroxymethyl)-(?) **10089-00-6**, Anthraquinone, 1,2,5,6,8-pentahydroxy-3-(hydroxymethyl)-(?)
(as structure of asperthecin)

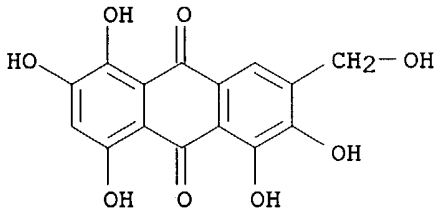
RN 481-68-5 CAPLUS

CN 9,10-Anthracenedione, 1,2,3,7,8-pentahydroxy-4-(hydroxymethyl)-(9CI) (CA INDEX NAME)



RN 10089-00-6 CAPLUS

CN 9,10-Anthracenedione, 1,2,5,6,8-pentahydroxy-3-(hydroxymethyl)-(9CI) (CA INDEX NAME)



(structure of, and derivs.

L12 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1956:39268 CAPLUS

DOCUMENT NUMBER: 50:39268

ORIGINAL REFERENCE NO.: 50:7590f-h

TITLE: Ultraviolet spectra of hydroxyanthraquinones

AUTHOR(S): Ikeda, Tetsutaro; Yamamoto, Yuzuru; Tsukida, Kiyoshi; Kanatomo, Shoichi

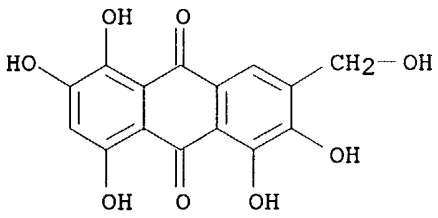
CORPORATE SOURCE: Univ. Kanazawa
SOURCE: Yakugaku Zasshi (1956), 76, 217-20
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB In the ultraviolet spectra of hydroxyanthraquinone derivs. (I), the absorption appearing in shorter wave region than 2500 A. is important. When anthraquinones have 1, 2, 3, and 4 OH groups, γmaximum appears at 2225, 2250, 2300 ± 25, and 2360 A., resp. These maximum are independent of the nature of OH groups, as at α or β, but the intensity value depends chiefly on the number of α-OH groups. The intensity of maximum absorption at about 2700 A. depends on the β-OH group; the log ε value above 4.1 shows the presence of a βOH group and the value below 4.1 indicates its absence. Thus, it would be possible to predict the number of OH groups and their α:β ratio from the ultraviolet absorption curve. Further, I with 1,4-di-OH groups in the mol. exhibit a shift in the visible region; the absorption maximum appears above 4800 A.

IT **10089-00-6**, Asperthecin
(spectrum of)

RN 10089-00-6 CAPLUS

CN 9,10-Anthracenedione, 1,2,5,6,8-pentahydroxy-3-(hydroxymethyl)- (9CI) (CA INDEX NAME)



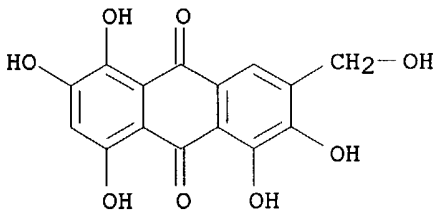
L12 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1955:46653 CAPLUS
DOCUMENT NUMBER: 49:46653
ORIGINAL REFERENCE NO.: 49:9084a-h
TITLE: Biochemistry of microorganisms. XCIV. The coloring matters of species in the Aspergillus nidulans groups. 1. Asperthecin, a crystalline coloring matter of Aspergillus quadrilineatus
AUTHOR(S): Howard, B. H.; Raistrick, H.
CORPORATE SOURCE: Univ. London
SOURCE: Biochemical Journal (1955), 59, 475-84
CODEN: BIJOAK; ISSN: 0264-6021
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 48, 10834i; 49, 1032c. The purple-red coloring matter of the perithecia and ascospores of 2 strains of A. quadrilineatus has been crystallized and named asperthecin (I). The mycelium of a 5-week old culture incubated at 24° was washed and homogenized in aqueous N HCl in a high-speed blendor. The resulting suspension was

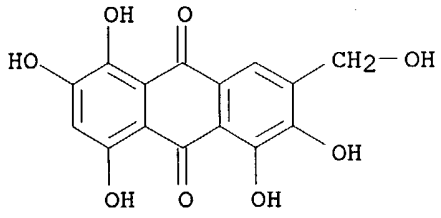
filtered, washed with water, and residue extracted with cold absolute EtOH. The orange-brown extract was partially evaporated in vacuo and gave crude I. Purification of I was accomplished by converting the crude I to the crystalline hexaacetate derivative (II), which was then hydrolyzed by refluxing in MeOH containing 3% (volume/volume) concentrated H_2SO_4. The recovered I then crystallized from MeOH or from dioxane with solvent of crystallization I with the formula $C_{15}H_{10}O_8$, darkens but does not melt at 370°, contains no OCH_3 or Me group attached to C, is insol. in H_2O, slightly soluble in organic solvents, soluble in pyridine (forming a pyridine salt which seps. on standing). I is reddish-orange in solns. of organic solvents and glacial HOAc, intensely purple in cold concentrated H_2SO_4, but does not fluoresce in daylight. I gives a stable purple ferric color in EtOH, is soluble in dilute $NaHCO_3$, Na_2CO_3 and NaOH, giving purple-red to purple solns. which are increasingly unstable in air with rise in pH and fade rapidly. The K salt is formed as a precipitate in EtOH with the addition of KOAc. I is chromatographically homogeneous, reduced by Zn dust in glacial HOAc to a pale yellow compound II ($C_{15}H_4O_2(OCOCH_3)_6$) was prepared by heating I with acetic anhydride containing 1.9% (volume/vol) H_2SO_4 and crystallized from EtOH as yellow crysts., m.p. 228°. II shows no optical activity in $CHCl_3$, is insol. in 0.5N $NaHCO_3$ and Na_2CO_3, gives no ferric color in EtOH. Pentamethyl-I ($C_{15}H_5O_3(OCH_3)_5$) (III) was prepared by refluxing a mixture of I, dry acetone, dimethylsulfate and freshly ignited K_2CO_3; m.p. 134-135°. III is insol. in alkali, gives a stable purple-blue solution in concentrated H_2SO_4 and a red solution in concentrated HNO_3. Dimethylasperthecin ($C_{15}H_8O_6(OCH_3)_2$) (IV) was prepared by brief methylation with diazomethane in acetone and crystallized from dioxane and then EtOH as bright red blades, m.p. 236-237°. IV is soluble in N Na_2CO_3, insol. in $NaHCO_3$, soluble in N NaOH (blue), concentrated H_2SO_4 (purple-blue), concentrated HNO_3 (blue), EtOH-$FeCl_3$ (purple-brown). IV is reduced by $Na_2S_2O_4$ to yield an orange-yellow solution in ether with green fluorescence. I is not reduced by $Na_2S_2O_4$. Dimethyl-I tetraacetate ($C_{15}H_4O_2(OCH_3)_2(OCOCH_3)_4$) (V) was prepared by acetylation of IV with acetic anhydride containing 2% (volume/volume) concentrated H_2SO_4 at 100°. V appeared as crystals of yellow rods which were washed with glacial HOAc and H_2O, m.p. 229-230°. V was hydrolyzed by refluxing with H_2SO_4-MeOH. Degradation of I by Zn dust yielded 2-methylanthracene, by HI and red P yielded Frangula emodin (4,5,7-trihydroxy-2-methylanthraquinone). It is concluded that I must be either 3,4,5,6,7- or 1,4,5,6,7-pentahydroxy-2-hydroxymethylanthraquinone. The position of the OH groups is inferred from a consideration of the absorption spectral properties of I. The infrared spectrum of solid I has a broad absorption band in the double-bond stretching region with a maximum at 1606 and a shoulder at 1575 cm.-1 I is a powerful mordant dyestuff and dyes white wool, mordanted with Cr, Al, or Ti an intense indigo blue, deep violet or dull red, resp. Evidence is presented that I is the coloring matter which is characteristic of the purple-red perithecia and ascospores of a number of other species of the A. nidulans group.

IT **10089-00-6**, Asperthecin

(preparation of)
RN 10089-00-6 CAPLUS
CN 9,10-Anthracenedione, 1,2,5,6,8-pentahydroxy-3-(hydroxymethyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1954:78333 CAPLUS
DOCUMENT NUMBER: 48:78333
ORIGINAL REFERENCE NO.: 48:13822e-f
TITLE: Pigments of the lower fungi (molds)
AUTHOR(S): Smith, George
CORPORATE SOURCE: School Hyg. Trop. Med., London
SOURCE: Congr. intern. botan., Paris, Rapps. et communs. (1954), 8(Sect. 18-20), 83-9
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The pigment responsible for the intense color of the perithecia of Aspergillus nidulans is hydroxymethylpentahydroxyanthraquinone, and has been named asperthecin. The general subject of mold pigments and their possible physiol. role is reviewed.
IT **10089-00-6**, Asperthecin
(in Aspergillus nidulans)
RN 10089-00-6 CAPLUS
CN 9,10-Anthracenedione, 1,2,5,6,8-pentahydroxy-3-(hydroxymethyl)- (9CI) (CA INDEX NAME)



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L13 3 S L11

L13 ANSWER 1 OF 3 CAOLD COPYRIGHT 2004 ACS on STN
AN CA58:6759e CAOLD
TI synthesis of polyhydroxyanthraquinones related to asperthecin
AU Birkinshaw, John H.; Gourlay, R.

IT 88856-64-8 92103-85-0 92439-41-3 **92439-43-5** 93994-00-4
94303-40-9 94385-93-0 94968-43-1 95125-38-5 95803-62-6
97081-05-5 97081-14-6 98862-11-4

L13 ANSWER 2 OF 3 CAOLD COPYRIGHT 2004 ACS on STN
AN CA56:8653i CAOLD
TI biochemistry of microorganisms - (CIX) structure of asperthecin
AU Birkinshaw, John H.; Gourlay, R.
IT 842-44-4 1206-37-7 3571-23-1 5924-63-0 6409-75-2
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75507-53-8 75507-56-1 75534-86-0 75534-87-1 88856-63-7
92103-84-9 92429-68-0 92429-99-7 93012-76-1 93994-09-3
95161-02-7 95225-44-8 95281-19-9 96060-74-1 96271-95-3
96578-47-1 97015-80-0 97081-12-4 100338-47-4

L13 ANSWER 3 OF 3 CAOLD COPYRIGHT 2004 ACS on STN
AN CA52:1131a CAOLD
TI microorganisms - (CI) coloring matters of species of the Aspergillus nidulans group (2) structure of asperthecin
AU Neelakantan, S.; Pocker, A.; Raistrick, H.
IT **481-68-5** 5953-90-2 **10089-00-6** 62554-73-8
103988-64-3 103989-81-7 109844-54-4 109844-55-5 111034-57-2
111527-63-0 112223-11-7 112223-13-9

FILE 'USPATFULL' ENTERED AT 11:23:32 ON 27 JUL 2004
L14 3 S L11

L14 ANSWER 1 OF 3 USPATFULL on STN
ACCESSION NUMBER: 2004:152139 USPATFULL
TITLE: Antihelminthic anthraquinones and method of use thereof
INVENTOR(S): Cichewicz, Robert H., Santa Cruz, CA, UNITED STATES
Nair, Muraleedharan G., Okemos, MI, UNITED STATES
McKerrow, James H., San Francisco, CA, UNITED STATES
PATENT ASSIGNEE(S): Board of Trustees of Michigan State University, East Lansing, MI, 48824-1046 (U.S. corporation)
The Regents of the University of California, Oakland, CA, 94607-5200 (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004116361	A1	20040617
APPLICATION INFO.:	US 2003-723672	A1	20031126 (10)
RELATED APPLN. INFO.:	Division of Ser. No. US 2002-317906, filed on 12 Dec 2002, PENDING		

	NUMBER	DATE
PRIORITY INFORMATION:	US 2002-372576P	20020415 (60)
	US 2002-389368P	20020617 (60)

Searcher : Shears 571-272-2528

NUMBER OF DRAWINGS: 7 Drawing Page(s)
LINE COUNT: 1696
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Anthraquinones are described which are antihelminthic and in particular, are useful in compositions for inhibiting Schistosoma sp. in vitro or in vivo. The preferred anthraquinones have the formula: ##STR1##

wherein R.sub.1, R.sub.2, R.sub.3, and R.sub.4 are each hydrogen, hydroxy, halogen, alkyl, substituted alkyl, alkene, substituted alkene, alkyne, aryl, substituted aryl, cyclic, substituted cyclic, acid group, carbohydrate, or combination thereof, R is a group containing 1 to 12 carbons such as methyl, alkyl, substituted alkyl, aldehyde, hydroxy, hydroxymethyl, acid group, carbohydrate, or combination thereof, and the halogen is I, F, Br, or Cl.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L14 ANSWER 3 OF 3 USPATFULL on STN
ACCESSION NUMBER: 2003:325050 USPATFULL
TITLE: Antihelminthic anthraquinones and method of use thereof
INVENTOR(S): Cichewicz, Robert H., Santa Cruz, CA, UNITED STATES
Nair, Muraleedharan G., Okemos, MI, UNITED STATES
McKerrow, James H., San Francisco, CA, UNITED STATES
PATENT ASSIGNEE(S): Board of Trustees of MICHIGAN STATE UNIVERSITY, East Lansing, MI (U.S. corporation)
The Regents of the University of California, Oakland, CA (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2003229032	A1	20031211	
APPLICATION INFO.:	US 2002-317906	A1	20021212	(10)

	NUMBER	DATE
PRIORITY INFORMATION:	US 2002-372576P	20020415 (60)
	US 2002-389368P	20020617 (60)

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: MCLEOD & MOYNE, P.C., 2190 COMMONS PARKWAY, OKEMOS, MI, 48864
NUMBER OF CLAIMS: 33
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 7 Drawing Page(s)
LINE COUNT: 1696
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Anthraquinones are described which are antihelminthic and in particular, are useful in compositions for inhibiting Schistosoma sp. in vitro or in vivo. The preferred anthraquinones have the formula: ##STR1##

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: MCLEOD & MOYNE, P.C., 2190 COMMONS PARKWAY, OKEMOS, MI, 48864
NUMBER OF CLAIMS: 33
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 7 Drawing Page(s)
LINE COUNT: 1694
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Anthraquinones are described which are antihelminthic and in particular, are useful in compositions for inhibiting Schistosoma sp. in vitro or in vivo. The preferred anthraquinones have the formula: ##STR1##

wherein R.sub.1, R.sub.2, R.sub.3, and R.sub.4 are each hydrogen, hydroxy, halogen, alkyl, substituted alkyl, alkene, substituted alkene, alkyne, aryl, substituted aryl, cyclic, substituted cyclic, acid group, carbohydrate, or combination thereof, R is a group containing 1 to 12 carbons such as methyl, alkyl, substituted alkyl, aldehyde, hydroxy, hydroxymethyl, acid group, carbohydrate, or combination thereof, and the halogen is I, F, Br, or Cl.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L14 ANSWER 2 OF 3 USPATFULL on STN
ACCESSION NUMBER: 2004:139510 USPATFULL
TITLE: Antihelminthic anthraquinones and method of use thereof
INVENTOR(S): Cichewicz, Robert H., Santa Cruz, CA, UNITED STATES
Nair, Muraleedharan G., Okemos, MI, UNITED STATES
McKerrow, James H., San Francisco, CA, UNITED STATES
PATENT ASSIGNEE(S): Board of Trustees of Michigan State University, East Lansing, MI (U.S. corporation)
The Regents of the University of California, Oakland, CA (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004106686	A1	20040603
APPLICATION INFO.:	US 2003-723671	A1	20031126 (10)

RELATED APPLN. INFO.: Division of Ser. No. US 2002-317906, filed on 12 Dec 2002, PENDING

	NUMBER	DATE
PRIORITY INFORMATION:	US 2002-372576P	20020415 (60)
	US 2002-389368P	20020617 (60)

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: MCLEOD & MOYNE, P.C., 2190 COMMONS PARKWAY, OKEMOS, MI, 48864
NUMBER OF CLAIMS: 33
EXEMPLARY CLAIM: 1

wherein R.sub.1, R.sub.2, R.sub.3, and R.sub.4 are each hydrogen, hydroxy, halogen, alkyl, substituted alkyl, alkene, substituted alkene, alkyne, aryl, substituted aryl, cyclic, substituted cyclic, acid group, carbohydrate, or combination thereof, R is a group containing 1 to 12 carbons such as methyl, alkyl, substituted alkyl, aldehyde, hydroxy, hydroxymethyl, acid group, carbohydrate, or combination thereof, and the halogen is I, F, Br, or Cl.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

(FILE 'MEDLINE, BIOSIS, EMBASE' ENTERED AT 11:23:53 ON 27 JUL 2004)
L15 1 S L11

L15 ANSWER 1 OF 1 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
ACCESSION NUMBER: 1987:138559 BIOSIS
DOCUMENT NUMBER: PREV198732067194; BR32:67194
TITLE: SECONDARY METABOLITES AS AN AID TO EMERICELLA CLASSIFICATION.
AUTHOR(S): FRISVAD J C [Reprint author]
CORPORATE SOURCE: FOOD TECHNOLOGY LABORATORY, TECHNICAL UNIVERSITY OF DENMARK, 2800 LYNGBY, DENMARK
SOURCE: NATO ASI Series Series A Life Sciences, pp. 437-444. SAMSON, R. A. AND J. I. PITT (ED.). NATO ASI (ADVANCED SCIENCE INSTITUTES) SERIES SERIES A: LIFE SCIENCES, VOL. 102. ADVANCES IN PENICILLIUM AND ASPERGILLUS SYSTEMATICS; FIRST INTERNATIONAL WORKSHOP, AMSTERDAM, NETHERLANDS, MAY 6-10, 1985. X+483P. PLENUM PRESS: NEW YORK, NEW YORK, USA; LONDON, ENGLAND. ILLUS. 1985 (RECD. 1986). Publisher: Series: NATO ASI Series Series A Life Sciences.
ISSN: 0258-1213. ISBN: 0-306-42222-0.
DOCUMENT TYPE: Book
Conference; (Meeting)
FILE SEGMENT: BR
LANGUAGE: ENGLISH
ENTRY DATE: Entered STN: 14 Mar 1987
Last Updated on STN: 14 Mar 1987

FILE 'HOME' ENTERED AT 11:24:03 ON 27 JUL 2004